```
STN Search — 10597445


=> d his

     (FILE 'HOME' ENTERED AT 10:30:43 ON 14 MAR 2008)

     FILE 'REGISTRY' ENTERED AT 10:30:50 ON 14 MAR 2008
L1              STRUCTURE UPLOADED
L2          0 S L1
L3         17 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 10:31:47 ON 14 MAR 2008
L4         19 S L3
L5         19 S L4 AND PY<=2006

     FILE 'REGISTRY' ENTERED AT 10:45:37 ON 14 MAR 2008
L6              STRUCTURE UPLOADED
L7          0 S L6
L8         14 S L6 FULL

     FILE 'REGISTRY' ENTERED AT 10:46:50 ON 14 MAR 2008

     FILE 'CAPLUS' ENTERED AT 10:46:53 ON 14 MAR 2008
L9         10 S L8

     FILE 'REGISTRY' ENTERED AT 10:54:53 ON 14 MAR 2008
L10             STRUCTURE UPLOADED
L11         6 S L10
L12       125 S L10 FULL

     FILE 'CAPLUS' ENTERED AT 10:56:13 ON 14 MAR 2008
L13        19 S L12

=> d stat que
L10             STR
```
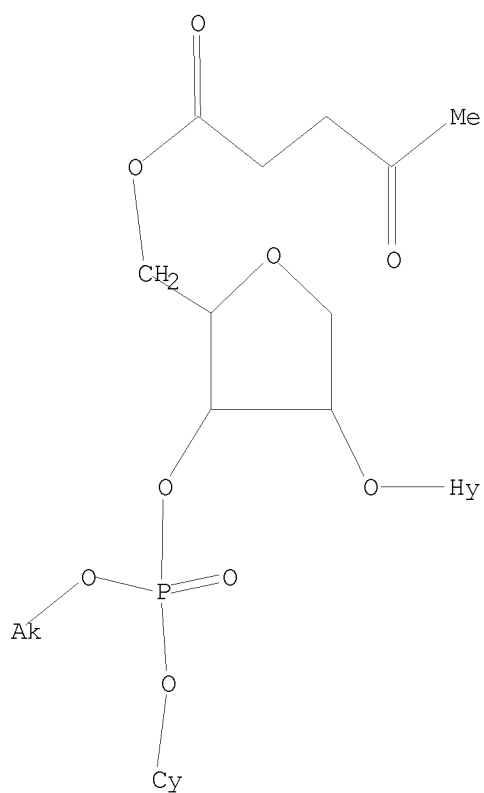
Structure attributes must be viewed using STN Express query preparation.
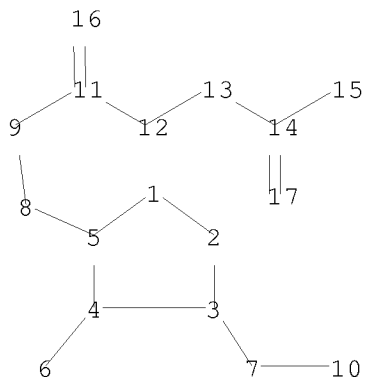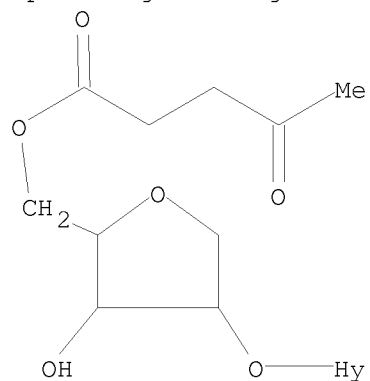L12   125 SEA FILE=REGISTRY SSS FUL L10
L13   19 SEA FILE=CAPLUS ABB=ON PLU=ON L12

STN Search - 10597445

=>
Uploading C:\Program Files\Stnexp\Queries\10597445-14Mar08-1.str

chain nodes :
6 7 8 9 10 11 12 13 14 15 16 17
ring nodes :
1 2 3 4 5
chain bonds :
3-7 4-6 5-8 7-10 8-9 9-11 11-12 11-16 12-13 13-14 14-15 14-17
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 3-7 4-5 4-6 7-10 9-11 11-16 14-17
exact bonds :
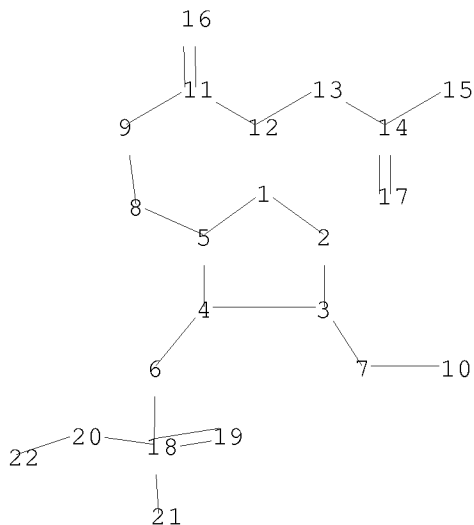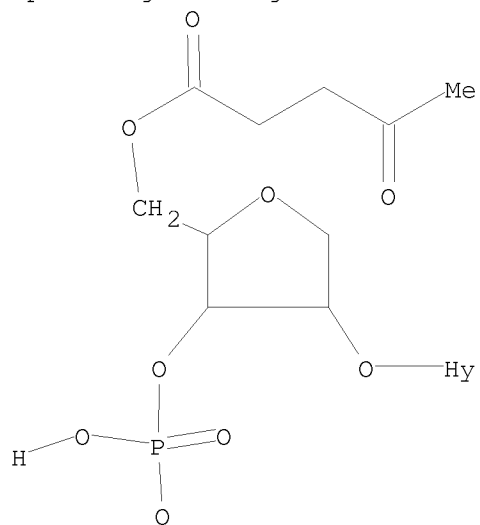5-8 8-9 11-12 12-13 13-14 14-15

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS

STN Search - 10597445

=>
Uploading C:\Program Files\Stnexp\Queries\10597445-14Mar08-.str

chain nodes :
6   7   8   9   10   11   12   13   14   15   16   17   18   19   20   21   22
ring nodes :
1   2   3   4   5
chain bonds :
3-7   4-6   5-8   6-18   7-10   8-9   9-11   11-12   11-16   12-13   13-14   14-15   14-17
18-19
18-20   18-21   20-22
ring bonds :
1-2   1-5   2-3   3-4   4-5
exact/norm bonds :
1-2   1-5   2-3   3-4   3-7   4-5   4-6   6-18   7-10   9-11   11-16   14-17   18-21
exact bonds :
5-8   8-9   11-12   12-13   13-14   14-15   20-22
normalized bonds :
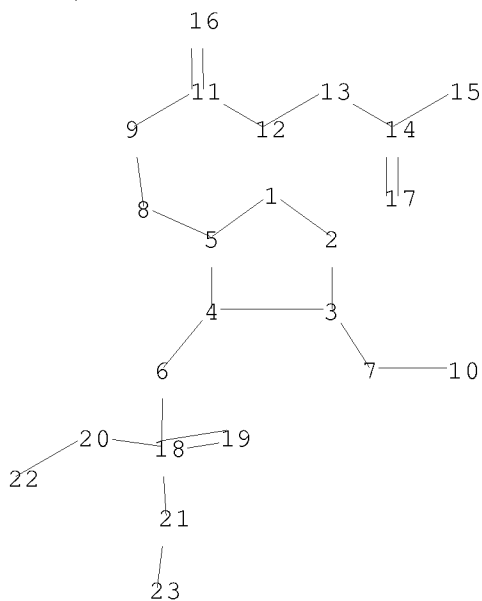18-19   18-20

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:CLASS   7:CLASS   8:CLASS   9:CLASS   10:Atom
11:CLASS   12:CLASS   13:CLASS   14:CLASS   15:CLASS   16:CLASS   17:CLASS   18:CLASS
19:CLASS   20:CLASS
21:CLASS   22:CLASS

=>
Uploading C:\Program Files\Stnexp\Queries\10597445-14Mar08-3.str

chain nodes :
6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
ring nodes :
1 2 3 4 5
chain bonds :
3-7 4-6 5-8 6-18 7-10 8-9 9-11 11-12 11-16 12-13 13-14 14-15 14-17
18-19
18-20 18-21 20-22 21-23
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 3-7 4-5 4-6 6-18 7-10 9-11 11-16 14-17 18-19 18-20
18-21 20-22 21-23
exact bonds :
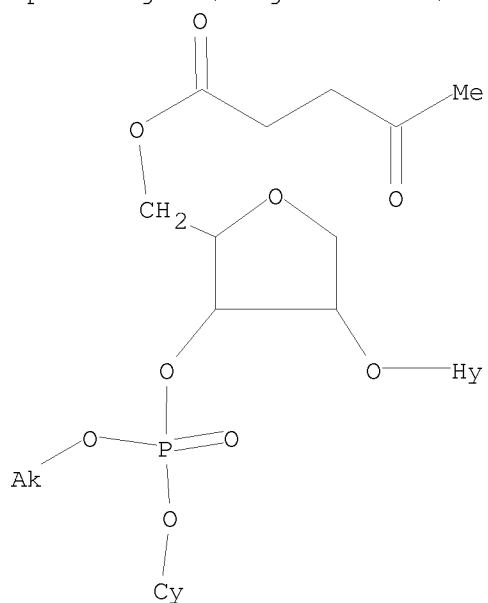5-8 8-9 11-12 12-13 13-14 14-15

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:Atom

STN Search - 10597445

=> d his

      (FILE 'HOME' ENTERED AT 07:52:07 ON 17 MAR 2008)

      FILE 'REGISTRY' ENTERED AT 07:52:22 ON 17 MAR 2008
                E LIPASE/CN
L1   1 S E3
L2   1 S E3 FULL

      FILE 'CAPLUS' ENTERED AT 07:52:53 ON 17 MAR 2008
L3   35400 S L2
L4   5363 S LEVULIN?
L5   104 S LEVULINOYL
L6   1327 S LEVULINATE
L7   4043 S LEVULINIC ACID
L8   4884 S L5 OR L6 OR L7
L9   1 S L2 (S) L8
L10   1 S L2 (L) L8
L11   16 S L2 AND L8

=> d stat que
L2   1 SEA FILE=REGISTRY ABB=ON PLU=ON LIPASE/CN
L5   104 SEA FILE=CAPLUS ABB=ON PLU=ON LEVULINOYL
L6   1327 SEA FILE=CAPLUS ABB=ON PLU=ON LEVULINATE
L7   4043 SEA FILE=CAPLUS ABB=ON PLU=ON LEVULINIC ACID
L8   4884 SEA FILE=CAPLUS ABB=ON PLU=ON L5 OR L6 OR L7
L11   16 SEA FILE=CAPLUS ABB=ON PLU=ON L2 AND L8

```
        FILE 'CASREACT' ENTERED AT 11:11:30 ON 20 MAR 2008
L1              STRUCTURE UPLOADED
L2          0 S L1
L3          0 S L2 FULL
L4          0 S L1 FULL
L5              STRUCTURE UPLOADED
L6          0 S L5
L7          0 S L5 FULL


        FILE 'STNGUIDE' ENTERED AT 11:14:52 ON 20 MAR 2008

        FILE 'REGISTRY' ENTERED AT 11:16:14 ON 20 MAR 2008
                E 2-CHLOROPHENYLPHOSPHOROTRIAZOLIDE
                E 2-CHLOROPHENYLPHOSPHOROTRIAZOLIDE/CN
                E PHOSPHOROTRIAZOLIDE/CN
L8       1668 S CHLORO (XA) PHOSPHORO (XA) PHENYL (XA) TRI
L9          0 S CHLORO (XA) PHOSPHORO (XA) PHENYL (XA) TRIAZOLIDE
L10       197 S CHLORO (XA) PHOSPHORO (XA) PHENYL (XA) TRIAZO?
L11       197 S CHLORO (XA) PHOSPHORO (XA) PHENYL (XA) TRIAZO? (XA) 2


        FILE 'CAPLUS' ENTERED AT 11:19:04 ON 20 MAR 2008
                E US2007172925/PN
L12         1 S E3


        FILE 'REGISTRY' ENTERED AT 11:20:45 ON 20 MAR 2008
L13         1 S 861817-06-3/RN
                SET NOTICE 1 DISPLAY
                SET NOTICE LOGIN DISPLAY


        FILE 'CAPLUS' ENTERED AT 11:21:40 ON 20 MAR 2008
                SEL L12 RN


        FILE 'REGISTRY' ENTERED AT 11:21:50 ON 20 MAR 2008
L14        85 S E1-E85
L15         3 S L14 AND PHOSPH?


        FILE 'CASREACT' ENTERED AT 11:22:47 ON 20 MAR 2008
L16        48 S L15


        FILE 'REGISTRY' ENTERED AT 11:26:25 ON 20 MAR 2008
L17         1 S L14 AND TRICHLORO?


        FILE 'CASREACT' ENTERED AT 11:27:09 ON 20 MAR 2008
L18       264 S L17
L19        48 S L18 AND PHOSPH?


        FILE 'CASREACT' ENTERED AT 11:40:02 ON 20 MAR 2008
L20         9 S L19 AND PHOSPHITE

        FILE 'STNGUIDE' ENTERED AT 11:50:16 ON 20 MAR 2008

=> d stat que
L14        85 SEA FILE=REGISTRY ABB=ON  PLU=ON  (100-07-2/BI OR 108-24-7/BI
                OR 109-78-4/BI OR 115-20-8/BI OR 118-00-3/BI OR 1191-99-7/BI
                OR 120187-92-0/BI OR 120187-94-2/BI OR 138494-30-1/BI OR
                21090-30-2/BI OR 40608-06-8/BI OR 40615-36-9/BI OR 40615-37-0/B
                I OR 40615-39-2/BI OR 64350-24-9/BI OR 65-46-3/BI OR 69304-37-6
                /BI OR 72351-28-1/BI OR 75-77-4/BI OR 79-30-1/BI OR 80817-46-5/
                BI OR 85393-37-9/BI OR 861816-91-3/BI OR 861816-92-4/BI OR
```

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                861816-93-5/BI OR 861816-94-6/BI OR 861816-95-7/BI OR 861816-97
                -9/BI OR 861816-98-0/BI OR 861816-99-1/BI OR 861817-01-8/BI OR
                861817-03-0/BI OR 861817-04-1/BI OR 861817-05-2/BI OR 861817-06
                -3/BI OR 861817-07-4/BI OR 861817-09-6/BI OR 861817-10-9/BI OR
                861817-11-0/BI OR 861842-82-2/BI OR 861842-83-3/BI OR 861842-85
                -5/BI OR 861842-86-6/BI OR 861842-87-7/BI OR 861842-88-8/BI OR
                861842-89-9/BI OR 861842-90-2/BI OR 861842-91-3/BI OR 861842-92
                -4/BI OR 861842-93-5/BI OR 861842-95-7/BI OR 861842-96-8/BI OR
                861842-97-9/BI OR 861842-98-0/BI OR 861842-99-1/BI OR 861843-00
                -7/BI OR 861843-01-8/BI OR 861843-02-9/BI OR 861843-03-0/BI OR
                861843-04-1/BI OR 861843-05-2/BI OR 861843-06-3/BI OR 861843-07
                -4/BI OR 861843-08-5/BI OR 861843-09-6/BI OR 861843-10-9/BI OR
                861843-11-0/BI OR 861843-12-1/BI OR 861843-13-2/BI OR 862202-73
                -1/BI OR 862224-10-0/BI OR 862224-11-1/BI OR 862224-12-2/BI OR
                862224-13-3/BI OR 862224-14-4/BI OR 862224-15-5/BI OR 862224-16
                -6/BI OR 862224-17-7/BI OR 862224-18-8/BI OR 862259-89-0/BI OR
                86327-76-6/BI OR 87865-78-9/BI OR 9001-62-1/BI OR 90865-73-9/BI
                OR 90865-74-0/BI)
L17          1 SEA FILE=REGISTRY ABB=ON  PLU=ON  L14 AND TRICHLORO?
L18        264 SEA FILE=CASREACT ABB=ON  PLU=ON  L17
L19         48 SEA FILE=CASREACT ABB=ON  PLU=ON  L18 AND PHOSPH?
L20          9 SEA FILE=CASREACT ABB=ON  PLU=ON  L19 AND PHOSPHITE
```
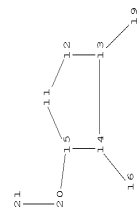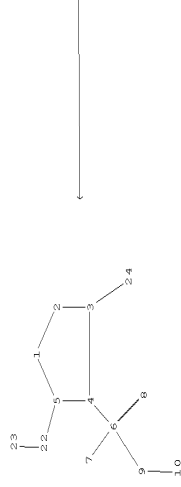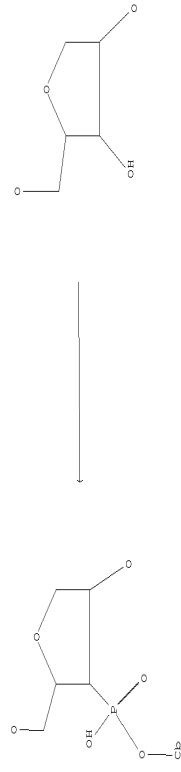
```
chain nodes :
  6   7   8   9   10   16   19   20   21   22   23   24
ring nodes :
  1   2   3   4   5   11   12   13   14   15
chain bonds :
  3-24   4-6   5-22   6-7   6-8   6-9   9-10   13-19   14-16   15-20   20-21   22-23
ring bonds :
  1-2   1-5   2-3   3-4   4-5   11-12   11-15   12-13   13-14   14-15
exact/norm bonds :
  1-2   1-5   2-3   3-4   3-24   4-5   6-9   11-12   11-15   12-13   13-14   13-19   14-15   14-16   20-21
  22-23
exact bonds :
  4-6   5-22   9-10   15-20
normalized bonds :
  6-7   6-8

Match level :
  1:Atom    2:Atom    3:Atom    4:Atom    5:Atom    6:CLASS   7:CLASS   8:CLASS   9:CLASS   10:Atom   11:Atom
  12:Atom   13:Atom   14:Atom   15:Atom   16:CLASS  19:CLASS  20:CLASS  21:CLASS  22:CLASS  23:CLASS
  24:CLASS
fragments assigned product role:
  containing 1
fragments assigned reactant/reagent role:
  containing 11
node mappings:
  4:14   4:14
```
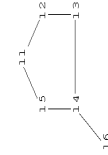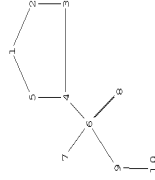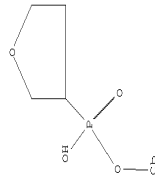
```
chain nodes :
  6  7  8  9  10  16
ring nodes :
  1  2  3  4  5  11  12  13  14  15
chain bonds :
  4-6  6-7  6-8  6-9  9-10  14-16
ring bonds :
  1-2  1-5  2-3  3-4  4-5  11-12  11-15  12-13  13-14  14-15
exact/norm bonds :
  1-2  1-5  2-3  3-4  4-5  6-9  11-12  11-15  12-13  13-14  14-15  14-16
exact bonds :
  4-6  9-10
normalized bonds :
  6-7  6-8

Match level :
  1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:CLASS   7:CLASS   8:CLASS   9:CLASS   10:Atom   11:Atom
  12:Atom  13:Atom  14:Atom  15:Atom  16:CLASS
reaction site bonds:
  4-6:XC  14-16:XC
```